ISBN: 978-3-95450-214-1 ISSN: 2673-5490 doi:10.18429/JACoW-IPAC2021-THPAB134

DEVELOPMENT AND ANALYSIS OF SOFTWARE FOR THE NUMERICAL SIMULATION OF FIELD EMISSION ELECTRON SOURCES*

N. S. Kakorin, N. V. Egorov, K. A. Nikiforov†
Saint Petersburg State University, St. Petersburg, Russia

Abstract

The open-source DAISI C++ package (Design of Accelerators, optImizations and SImulations) is extended with the ability to simulate the operation of electron sources in the field emission mode, with the user-defined initial distribution of emitted electrons velocities, as a model parameter, and with the automated calculation of current-voltage characteristics. Particles injection scheme is suggested. Computational experiments are performed for silicon carbide field emission electron source nanostructure with bimodal energy spectrum, revealed from experimental study, and comparative analysis with Maxwell distribution is presented.

INTRODUCTION AND MOTIVATION

It is extremely important for effective functioning of the field emission electron sources to prevent beam particles from getting to the forming electrodes. The greatest current-deposition danger comes from the particles located on the periphery of the beam. So it is an actual problem to improve approaches of simulation of the field emission electron sources, because the initial velocity distribution has a significant influence on the emission picture, but the simplest models are utilizing zero initial velocity spread or Maxwell distribution, that doesn't always match experimental data [1–3].

SOFTWARE DEVELOPMENT

In DAISI the particle-in-cell (PIC) method is split into two modules [3], one of which consists of solvers and the other is a software abstraction of the physical model. Calculation of current density with the Fowler-Nordheim model is being integrated into the solvers part and corresponding injection scheme with a user-defined initial velocity distribution is being realized in software abstraction of physical device. The exact modified parts are shown in the fragment of the UML class diagram (Fig. 1).

The physical model of the field emission electron source consists of the following assumptions: 1. The work function of the material is constant; 2. It is a quasi-electrostatic approximation with axial symmetry.

Two-dimensional computational domain $\overline{G} = G \cup \partial G$ is considered, where ∂G is boundary of domain and $\partial G = \partial G_1 \cup \partial G_1$. Poisson's equation is used to compute the electrostatic potential U pursuant to quasi-electrostatic approximation and in compliance with axial symmetry in Euler cylindrical coordinates (r, z) (according to axisymmetric electron source cell $\partial/\partial\varphi = 0$,

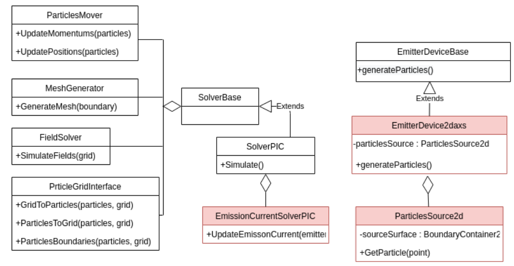

Figure 1: Fragment of the UML class diagram of DAISI implementation of PIC calculations and particle injection scheme. Red colored blocks show modified part of C++ code, which allow to simulate the operation of electron sources in the field electron emission mode, with the choice of the initial distribution of electron velocities.

where φ — azimuth coordinate):

$$\frac{\partial^2 U(r,z)}{\partial r^2} + \frac{\partial^2 U(r,z)}{\partial z^2} + \frac{1}{r}\frac{\partial U(r,z)}{\partial r} = -\frac{\rho(r,z)}{\varepsilon_0}, \quad (r,z) \in G, \quad (1)$$

$$E_r(r,z) = -\frac{\partial U(r,z)}{\partial r}, \quad E_z(r,z) = -\frac{\partial U(r,z)}{\partial z},$$

$$\begin{cases} U = g(r,z), & (r,z) \in \partial G_1, \\ \dfrac{\partial U}{\partial \vec{n}} = 0, & (r,z) \in \partial G_2, \end{cases} \quad (2)$$

where $\rho(r,z)$ — space charge density, ε_0 — electric constant, $g(r,z)$ — function that describes boundary potential, $\vec{n}$ — normal vector to the boundary ∂G_2 (axis of symmetry and side boundary of electron source cell). The motion of particles is described with reduced momentum p_r, p_z, p_z by following equations in Lagrangian cylindric coordinates (r, z) (for model macroparticles, the relativistic form of the equations of motion is used, taking into account the realization of the particle-in-cell method [3]):

$$\begin{cases} \dfrac{\mathrm{d}r}{\mathrm{d}\tau} = \dfrac{p_r}{\gamma}, & \dfrac{\mathrm{d}p_r}{\mathrm{d}\tau} = \dfrac{eE_r}{m_0 c^2} + \dfrac{p_\varphi^2}{r^3\gamma}, \\ \dfrac{\mathrm{d}z}{\mathrm{d}\tau} = \dfrac{p_z}{\gamma}, & \dfrac{\mathrm{d}p_z}{\mathrm{d}\tau} = \dfrac{eE_z}{m_0 c^2}, \\ & \dfrac{\mathrm{d}p_\varphi}{\mathrm{d}\tau} = 0, \end{cases} \quad (3)$$

$$(r(0), z(0)) \in \partial G_1, \quad (p_r(0), p_\varphi(0), p_z(0)) = \vec{p}_0, \quad (4)$$

where initial positions of particles are given on part of boundary ∂G_1 including emission area; $\gamma = \sqrt{1 + p_r^2 + p_z^2 + (p_\varphi/r)^2}$, $\tau = ct$, c — speed of light, m_0/q — ratio of rest mass to electron charge (model particles have the same ratio). Initial momentums

* Work supported by RFBR, project number 20-07-01086
† k.nikiforov@spbu.ru

ISBN: 978-3-95450-214-1 ISSN: 2673-5490 doi:10.18429/JACoW-IPAC2021-THPAB134

related with initial velocities v_0 that are given by Maxwell distribution or user-defined distribution (as described in next section), $\vec{p}_0 = \vec{v}_0 \gamma / c$.

Current density is determined according to the Fowler-Nordheim field emission model [1]:

$$j(E) = \frac{A(\beta_e E(s))^2}{t^2(y)\Phi} \exp\left(\frac{-B\Phi^{3/2}}{\beta_e E(s)} \nu(y)\right), \tag{5}$$

where $j(E)$ — current density (A/m^2 for E measured in V/m), Φ — work function of material (eV), β_e — local field enhancement factor [4, 5], $E(s)$ — magnitude of the field strength vector in point s, A and B — Fowler–Nordheim constants, y — Nordheim parameter, $\nu(y), t(y)$ — approximations of elliptic Nordheim functions found by Forbes and Deane that give a more accurate approximation in comparison with the classic Shmidt approach [6].

METHODS OF SIMULATION

Injection of particles is suggested by the following scheme:

1. Emission surface is represented as a partition of an interval in 2D space σ_N with the number of subparts equals N, which value depends on the grid.
2. Current density from the whole subpart is considered to be equal to current density calculated at the center point of the subpart.
3. Emission surface is represented as a partition of an interval in 2D space σ_K with the number of subparts equals $K < N$ and it is a model parameter.
4. Macroparticle is injected from the center of every subpart of the σ_K and current calculation is based on the current sum from all subparts of σ_N that are covered with considered σ_K subpart.

Additional partition of an interval σ_K is required because constructed grid according to Runge rule leads to too high value of N. DAISI computational algorithms perform particle injection at fixed points during the simulation. If particles will be injected from each subpart from σ_N then it will lead to very low performance and injected particles will carry a very small amount of charge, significantly lesser than elementary. To reduce the influence of N new smaller partition σ_K is introduced and it is used as an aggregator of current density from subparts of σ_N at one fixed point required for DAISI.

This scheme allows one to take into account the nontrivial specifics of the emission surface. And macroparticles that carry the most charge are matching surface regions with the highest current density. Also, it is should be noted that emission surface length is a model parameter. Let us introduce the probability density function (PDF) of the bimodal random variable based on the field electron emission energy distribution spectra (Fig. 2). Considering spectrum as a function of energy x it can be described as a piecewise linear function $g(x)$ that equals to spectrum value within obtained energy interval $[E_{spec,min}, E_{spec,max}]$ and zero otherwise, where $E_{spec,min}$, $E_{spec,max}$ — minimal and maximum spectrum

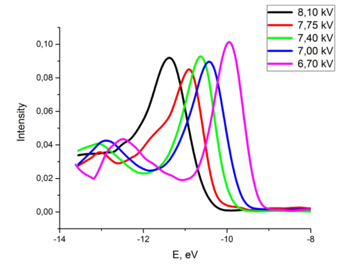

Figure 2: Energy distribution spectra of silicon carbide structures [7].

values. PDF can be obtained $f(x)$ after the normalization of the $g(x)$:

$$f(x) = k_{norm} g(x), \tag{6}$$

where k_{norm} is normalization factor. The cumulative distribution function now can be easily obtained integrating (6) on $(-\infty, x]$.

To simulate this random variable, the inverse function method based on uniform random numbers [8] is used, but because the spectrum is set for limited energy values $[E_{spec,min}, E_{spec,max}]$, the folowwing problem is to model the truncated distribution [8]. To simulate a truncated random variable on the segment $[a, b]$, it is necessary to obtain the values of the random numbers on the segment $F(a), F(b)$:

$$x = F^{-1}(R(F(E_{spec,min}), F(E_{spec,max}))). \tag{7}$$

The following equation can be solved with respect to x:

$$\gamma = F(x) = \int_{E_{spec,min}}^{x} f(y)dy, \tag{8}$$

where $\gamma \sim R(F(E_{spec,min}), F(E_{spec,max}))$. Considering $E_{spec,min} = x_1 < x_2 < ... < x_{N_{spec}} = E_{spec,max}$, where N_{spec} — number of value of the spectrum numerical representation, and because the integration nodes are fixed, and not equidistant, for the numerical approximation of the integral the trapezoid rule can be used:

$$\int_{E_{spec,min}}^{x} f(y)dy = \frac{1}{2}\sum_{j=2}^{i}(f(x_{j-1}) + f(x_j)) \cdot (x_j - x_{j-1}). \tag{9}$$

Combining Eqs. (9) and (8) with respect to i is obtained, from which the velocity of the particle can be expressed in explicit form using the particle's kinetic energy equation.

ANALYSIS OF THE RESULTS

The cell of a field emission array electron source with a blade structure of vertical type emitters [1] in a triode configuration is considered to illustrate capabilities of the software.

The surface of the emitter is modeled as an ideal conductor without a dielectric coating associated with the presence of adsorbates, the edge of the blade is approximated by the toroid surface with an elliptical section with semi-axes of the ellipse 120 and 50 nm.

ISBN: 978-3-95450-214-1 ISSN: 2673-5490 doi:10.18429/JACoW-IPAC2021-THPAB134

Computations are performed for two emission surfaces length 144 nm (Fig. 3) and 30 nm to eliminate influence of this model parameter. Both results (Fig. 4) are obtained with fixed σ_N and with σ_K for $K = 600, 1000$ to show that with additional σ_K partition of an interval there is no qualitative difference in simulation results.

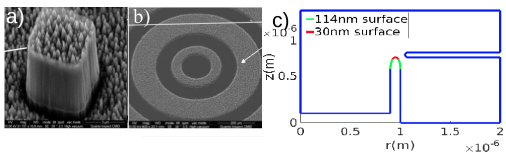

Figure 3: Silicon carbide nanostructures under the study [9–11]: a) SEM-image of field emission cell with razor-blade emitter; b) SEM-image of cylindrical blade structure [10]; c) geometric configuration of the electron source cell with two emission surface lengths — 144 nm (red and green combined) and 30 nm (red).

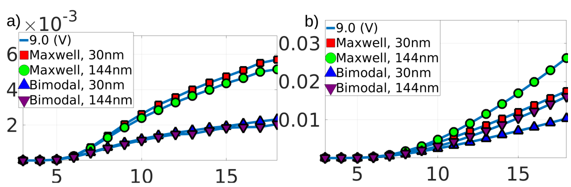

Figure 4: Pairwise comparison for both emission surface lengths: a) anode current from the gateway potential with bimodal and Maxwell initial velocity distribution; b) cathode current from the gateway potential with bimodal and Maxwell initial velocity distribution.

Influence of σ_K doesn't cause significant changes on simulation results for different K. Also, Maxwell distribution leads to the injection of particles that are faster and carry a lesser charge (Fig. 5).

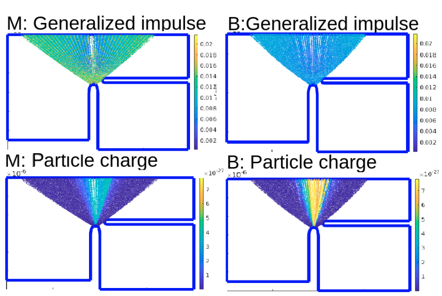

Figure 5: Pairwise comparison of the distribution of particles momentum (top pictures) and charge (bottom pictures) in the electrode gap for the Maxwell (left images) and bimodal (right images) initial distributions.

CONCLUSION

DAISI PIC code related to the calculation of the current density is extended with a field emission simulation, and injection of charged particles is extended with a such model parameter, as initial velocity distribution. Particle injection scheme was suggested and simulation results are obtained for the considered silicon carbide nanostructure as field emission electron source within the foregoing model assumptions. Simulated emission current collected on anode with bimodal initial velocity distribution approximately two times lesser than with Maxwell distribution with its parameter equals the expected value of the energy spectra.

ACKNOWLEDGEMENTS

Scientific research were performed at the Research park of St. Petersburg State University "Centre for Nanofabrication of Photoactive Materials (Nanophotonics)", "Interdisciplinary Center for Nanotechnology" and "Computing Center".

REFERENCES

[1] N. Egorov and E. Sheshin, *Field emission electronics*. International Publishing: Springer, 2017.

[2] K. L. Jensen, *Introduction to the physics of electron emission*, Hoboken, NJ, USA: John Wiley & Sons, 2017.

[3] V. Altsybeyev *et al.*, "Numerical simulation of a triode source of intense radial converging electron beam," *Journal of Applied Physics*, vol. 120, no. 14, p. 143301, Oct. 2016. doi:10.1063/1.4964335

[4] A. N. Zartdinov and K. A. Nikiforov, "Studying electric field enhancement factor of the nanostructured emission surface," *Journal of Physics: Conference Series*, vol. 741, p. 012006, Aug. 2016. doi:10.1088/1742-6596/741/1/012006

[5] Y. Feng and J. P. Verboncoeur, "A model for effective field enhancement for Fowler–Nordheim field emission," *Physics of Plasmas*, vol. 12, no. 10, p. 103301, Oct. 2005. doi:10.1063/1.2103567

[6] R. G. Forbes and J. H. Deane, "Reformulation of the standard theory of Fowler–Nordheim tunnelling and cold field electron emission," in *Proc. of the Royal Society A: Mathematical, Physical and Engineering Sciences*, Biggleswade, United Kingdom, Aug. 2007, pp. 2907–2927. doi:10.1098/rspa.2007.0030

[7] K. Nikiforov *et al.*, "The energy spectrum of field emission electrons from 4H silicon carbide," in *Proc. 33rd International Vacuum Nanoelectronics Conference (IVNC)*, Online, Jul. 2020, p. 9203525. doi:10.1109/ivnc49440.2020.9203525

[8] L. Devroye, *Non-uniform random variate generation*. New York City, NY, USA: Springer-Verlag, 1986.

[9] A. V. Afanasyev *et al.*, "Investigation of a possibility of development of a triode type electron field source based on 4H-SiC-structure with a semi-insulating epitaxial layer," *Nano- i Mikrosistemnaya Tehnika*, vol. 20, no. 12, pp. 719–726, Dec. 2018. doi:10.17587/nmst.20.719-726

[10] A. V. Afanasiev, *et al.*, "Family of silicon carbide solid state, vacuum and micromechanical switches for harsh environments," *Microwave Electronics and Microelectronics*, vol. 1, no. 1, pp. 80–84, 2017.

[11] M. A. Kuznetsova and V. V. Luchinin, "Focused ion beam machining of SiC field emitters," *Nano and Microsystems Technology*, vol. 12, no. 149, pp. 35–40, 2012.